

Progress Toward Affordable High Fidelity Combustion Simulations Using Filtered Density Functions for Hypersonic Flows in Complex Geometries

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Significant progress has been made in the development of subgrid scale (SGS) closures based on a filtered density function (FDF) for large eddy simulations (LES) of turbulent reacting flows. The FDF is the counterpart of the probability density function (PDF) method, which has proven effective in Reynolds averaged simulations (RAS). However, while systematic progress is being made advancing the FDF models for relatively simple flows and lab-scale flames, the application of these methods in complex geometries and high speed, wall-bounded flows with shocks remains a challenge. The key difficulties are the significant computational cost associated with solving the FDF transport equation and numerically stiff finite rate chemistry. For LES/FDF methods to make a more significant impact in practical applications a pragmatic approach must be taken that significantly reduces the computational cost while maintaining high modeling fidelity. An example of one such ongoing effort is at the NASA Langley Research Center, where the first generation FDF models, namely the scalar filtered mass density function (SFMDF) are being implemented into VULCAN, a production-quality RAS and LES solver widely used for design of high speed propulsion flowpaths. This effort leverages internal and external collaborations to reduce the overall computational cost of high fidelity simulations in VULCAN by: implementing the high order methods that allow reduction in the total number of computational cells without loss in accuracy; implementing first generation of high fidelity scalar PDF/FDF models applicable to high-speed compressible flows; coupling RAS/PDF and LES/FDF into a hybrid framework to efficiently and accurately model the effects of combustion in the vicinity of the walls; developing efficient Lagrangian particle tracking algorithms to support robust solutions of the FDF equations for high speed flows; and utilizing finite rate chemistry parametrization, such as flamelet models, to reduce the number of transported reactive species and remove numerical stiffness. This paper briefly introduces the SFMDF model (highlighting key benefits and challenges), and discusses particle tracking for flows with shocks, the hybrid coupled RAS/PDF and LES/FDF model, flamelet generated manifolds (FGM) model, and the Irregularly Portioned Lagrangian Monte Carlo Finite Difference (IPLMCFD) methodology for scalable simulation of high-speed reacting compressible flows.

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I. Introduction

Recent flight demonstrations of hypersonic air-breathing vehicles^{1,2} prove their increasing promise for military (rapid response and strike capability on global scale), aerospace (safer and more affordable access to space), and civil aviation (hypersonic transport) applications. Currently, these technologies are in their early development stages with commercial interest and internal research and development investment at a small fraction of that of government organizations such as National Aeronautics and Space Administration (NASA) and Air Force Research Laboratories (AFRL). To advance hypersonic air-breathing technologies to the technology readiness level (TRL) necessary for wide spread commercialization, further government investments are needed over the next decade and likely beyond. However, designing devices capable of robust hypersonic air-breathing operation, characterized by rapid mixing and short combustion times while ensuring flame stability, has proven difficult because the inherent high flow through velocities currently challenge both experimental and computational capabilities. In particular, current experimental facilities are sub-scale allowing for 1x-10x mass flow rates (with 1x equal to 10 lbm/sec of air flow) where 100x scale ups are needed. Flow diagnostics are typically limited to wall pressures and temperatures with non-intrusive, multi-dimensional, flow field information needed to advance knowledge and modeling. The current computational capabilities have shortcomings in both numerical methods (e.g. high order shock capturing) and physical models (e.g. compressible turbulence, turbulence-chemistry interaction, finite-rate kinetics) appropriate to these high velocity flow regimes.

Internal high-speed flows, such as those typically found in scramjet combustors, pose a particular challenge for computational fluid dynamics (CFD) because of complex, non-linear interactions between viscous wall-bounded flows, mixing layers, shocks, and thermodynamic and chemical non-equilibrium flow physics. More specifically, scramjet combustors are required to operate near optimum efficiency with minimal aerodynamic loss in flow regimes where flow and chemical time scales are of the same order. Therefore, the interactions of turbulence and finite-rate chemical kinetic effects will play a leading role in determining flow and flame characteristics and must be modeled with high fidelity. Such similarity of scale can also cause the flow regime to be highly unstable and susceptible to flame extinction and re-ignition phenomena which can have a detrimental impact on overall combustor operation and lead to a loss of thrust, narrowing of operability margins, and engine unstart. Unfortunately, due to these multi-scale, multi-physics interactions, this flow regime is also extremely challenging to model because no assumptions can be accurately postulated about the relationships between time and length scales of the multi-physics phenomena. Therefore, the dynamic interactions of multi-physics, multi-scale phenomena must be simulated rather than modeled.

The need for predictive simulation of multi-scale flows has led to the development of large eddy simulation (LES). In LES, the turbulence is separated into large-scale, grid-resolved, and geometry-influenced flow motions, and small-scale, unresolved but universally-behaving modeled motions.³ This “divide-and-conquer” approach utilizes brute force computing to resolve the most challenging dynamical interactions of the flow and relies on “sub-grid” models for the more universal small-scale flows. Because of this, LES is inherently unsteady and computationally expensive. Nevertheless, significant advancements in computational hardware, numerical algorithms, and physics models over the last two decades have increased our ability to employ LES for the unsteady simulation of reacting flows in practical devices.^{4,5} LES also offers a substantial computational cost reduction over direct numerical simulation (DNS). This cost reduction is proportional to the cube power of the sub-grid Reynolds number, Re_{Δ} .⁶ The value of the sub-grid Reynolds number for a typical LES of practical interest varies from 10-100 (or more) depending on the characteristic flow Reynolds number. This represents a dramatic three-to-six orders of magnitude computational cost reduction that makes LES of practical systems possible and the corresponding DNS difficult to imagine in the foreseeable future. Fortunately, numerical algorithm requirements for both LES and DNS are the same; therefore any tools developed for LES are directly applicable for DNS. The latter can then be used to elucidate physical interactions in computationally accessible canonical problems⁷⁻¹⁰ which can further lead to the development of improved physics models.

Not all physical phenomena, however, bear strong functional dependence on the LES-resolved multi-scale dynamics. While the LES predictions of geometry-governed mixing processes, such as swirling, recirculation, or vortex breakdown, are greatly improved over those using Reynolds averaged simulations (RAS), the prediction of turbulent-reacting flows remains a challenge. This is because combustion phenomena in both premixed and non-premixed systems takes place when the reactants experience transport at the molecular level (i.e. sub-grid). For example, in non-premixed systems, the LES-resolved processes only serve to “wrinkle and strain” the interface between the reactants thereby increasing the contact surface area. While accurate prediction of the total “contact” area is important for combustion, only the action of molecular diffusion mixes the reactants in a way that enables chemical reactions to occur. Similarly, for premixed combustion, the turbulent stirring processes only “move around” cold premixed pockets

of fuel and oxidizer, whereas it is the molecular thermal diffusion (diffusion of heat away from the reaction zone and into the unburned pockets of the mixture) that increases the temperature of the premixed reactants to levels required for self-sustained chemical reactions. As suggested above, both molecular and thermal diffusion are transport processes that directly influence chemical reactions. But since they occur at the smallest turbulent length scales (dissipation scales), they are unresolved in LES. This implies that the advantages of LES over RAS do not fully apply in turbulent *reacting* flows.

The fact that the benefits of LES over RAS cannot be effectively realized in reacting flows is disappointing but should not be discouraging. This is because over the past forty years researchers have been actively developing turbulence-chemistry interaction models for reacting RAS. The successes achieved by RAS modelers provide confidence in continued use of RAS in design and justify further development of models. Furthermore, given that challenges associated with turbulence-chemistry interaction modeling are comparable between LES and RAS, the experience gained during RAS development can be directly leveraged to develop corresponding models for LES. This strategy has been effectively used during the last twenty years.

The majority of current models for turbulence-chemistry interaction for LES (and RAS) are based on statistical approaches. A few exceptions are models based on deconvolution,^{11–13} fractal dynamics,^{14,15} and stochastic descriptions of the structure of turbulence dynamics.^{16,17} Reviews of turbulent combustion modeling for LES of low-speed and high-speed flows are provided by Pitsch,¹⁸ and Drummond,¹⁹ respectively. The commonly used statistical models define a joint probability density function (PDF) of density, reacting scalars, temperature, pressure (for high-speed flows), and certain turbulence quantities such as turbulence mixing frequency. The primary benefit of PDF-based models is that the averaged, or filtered, chemical reaction terms appear in a closed form. This is not a trivial accomplishment because, as argued in the previous paragraph, the chemical reactions are unresolved by LES. Furthermore, the closed-form model for the chemical reactions allows for dynamic coupling between the sub-grid and resolved processes thereby promising significant improvements in predictive fidelity. The simplest of PDF models assume the shape and nature of statistical relationships (e.g. statistical independence) among the state variables.^{20,21} Higher fidelity models, however, rely on solving transport equations governing those shapes and statistical relationships.^{22–31} This class of models, termed filtered density function (FDF) to distinguish them from PDF-based models used in RAS, has proven effective for LES of reacting flows.^{5,28,32,33} In this paper, the Lagrangian version of the joint scalar (composition) FDF (SFDF) is considered for applications in high speed flows. While the understanding and acceptance of the FDF methods for combustion simulations have been growing and versions of the models have been implemented in commercial software products, their use for cases of practical interest has been limited. This is mainly due to computational costs associated with solving the FDF transport equations in complex three-dimensional (3D) flow configurations that are now commonly utilized for design. Therefore, just as improvements to algorithms for solutions of Navier-Stokes equations greatly contributed to reduction of overall computational cost, improvements to algorithms for solutions of the FDF are expected to have a similar impact.

The computational costs of turbulence-chemistry interaction models are further increased by the numerical cost of evaluating of detailed, physics-based molecular diffusion and finite-rate chemical kinetics models.³⁴ The former describes the molecular diffusion phenomena which, as discussed above, are paramount to (sub-grid) molecular mixing processes leading to sustained chemical reactions. The latter describes rates of conversion processes that recombine fuel and oxidizer species into combustion products. This paper focuses on techniques used to reduce the computational cost of finite-rate chemical kinetics models with four dimensional (three spatial dimensions and time) simulations in mind. This is because it is widely recognized that the numerical computations of chemical reactions represent a large fraction of total simulation cost. In general, each species component deemed important for accuracy of a reacting simulation requires the solution of a transport equation. Even for simple fuels, such as hydrogen,³⁵ this requirement alone can result in a large number of transport equations as compared to non-reacting flows. However, it is not only the increase in the total number of transport equations that poses a great challenge. The number of rate expressions required for evaluation of the species' chemical source terms is typically about five times that of the number of species.³⁴ Additionally, those rate expressions often involve complicated, non-linear functions or algebraic expressions that include exponential, products of scalar variables raised to non-integer powers, and contain a disparate range of time scales resulting in stiffness. The stiffness, in particular, poses a challenge for numerical time integration algorithms. Combined, these challenges are so great that some of the most accurate detailed chemical kinetics mechanisms that include pollutant formation details (e.g. NO_x chemistry), containing thousands of species and tens-of-thousands of rate coefficients, can only be used within zero (e.g. perfectly stirred reactor) or one-dimensional (e.g. opposed flow flames) simulations. However, attempts at addressing computational issues related to efficiently solving detailed reacting systems may be in vain if the accuracy of the chemical kinetics mechanism to

predict key combustion phenomena, such as ignition delay time and flame propagation speed, is not improved. This is especially important in high speed propulsion applications where optimal combustion efficiency is often achieved in combustion regimes at low-to-moderate pressures (0.5-5 atm) and, because of high flow velocities, the combustion is increasingly sensitive to both ignition delay time and flame propagation speed.

Given the availability of accurate chemical kinetics mechanisms, the numerical costs associated with integrating a large number of stiff transport equations containing complicated source terms can be lowered by reducing the number of transport equations, accelerating rate calculations, and removing stiffness. A detailed discussion of current state-of-the-art is presented in Lu and Law.³⁴ One promising technique that offers to address the three challenges outlined above is the flamelet generated manifold (FGM) model.³⁶ This model considers a tabulated chemistry parametrization technique that reduces a total number of species to a much smaller number of important progress variables (for which transport equations must be solved and which parametrize all other species). Simultaneously, it is possible to pre-compute and pre-integrate the chemical source terms as a function of progress variables to avoid the costly on-the-fly reaction rate evaluations and stiff integration. Theoretically, the accuracy of the model approaches that of the detailed chemical kinetic scheme from which it is derived in the limit of number of progress variables approaching the number of species. The numerical implementations of FGM must include construction of an efficient table lookup/interpolation algorithm. The main benefit of tabulated chemistry frameworks is the flexibility to incorporate practical experience about important processes and parameters into the definitions of the parametrization and weigh fidelity (i.e. number of progress variables) against computational cost. When detailed chemical kinetic predictions are beyond computational feasibility, both of these elements allow for a pragmatic approach to simulations of reacting flows that offer major improvements over the current state-of-the-art.

II. Compressible FDF formulation for first generation models

The following section describes the mathematical formulation of the first generation of FDF-based high fidelity models for the turbulence-chemistry interactions in LES of high speed flows. The current formulation is based on the mass-weighted SFDF, termed the joint scalar filtered mass density function (SFMDF), developed for LES of low-speed reacting flows by Jaber et al.³⁷ The SFMDF is further modified to account for the compressibility effects following the RAS/PDF work of Hsu et al.³⁸

A. Governing Equations

Implementation of LES involves the use of the spatial filtering operation³

$$\langle Q(\mathbf{x}, t) \rangle_\ell = \int_{-\infty}^{+\infty} Q(\mathbf{x}', t) \mathcal{G}(\mathbf{x}' - \mathbf{x}) d\mathbf{x}' \quad (1)$$

where $\mathcal{G}$ denotes the temporally invariant, localized, symmetric, and positive filter kernel of width Δ_L , and $\langle Q(\mathbf{x}, t) \rangle_\ell$ represents the filtered value of the transport variable $Q(\mathbf{x}, t)$. In variable density flows it is convenient to consider the Favré filtered quantity, $\langle Q(\mathbf{x}, t) \rangle_L = \langle \rho Q \rangle_\ell / \langle \rho \rangle_\ell$.

The flow field to be simulated is unsteady, three-dimensional (3D), and involves gaseous (single-phase) combustion. Newton's law of viscosity, Fourier's law of heat conduction and Fick's law of mass diffusion are employed. The caveats in the use of these laws in reacting flows are recognized.³⁹ The primary transport variables are the fluid density ρ , the velocity vector u_i , $i = 1, 2, 3$ along the x_i direction and at a time t , the pressure p , the mass fractions of n_s species, Y_α ($\alpha = 1, 2, \dots, n_s$), and the sensible enthalpy h^s .

The transport variables satisfy the conservation equations of mass, momentum, species' mass fractions, and enthalpy. The filtered form of these equations is:

$$\frac{\partial \langle \rho \rangle_\ell}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L}{\partial x_i} = 0 \quad (2)$$

$$\frac{\partial \langle \rho \rangle_\ell \langle u_j \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L \langle u_j \rangle_L}{\partial x_i} = - \frac{\partial \langle p \rangle_\ell}{\partial x_j} + \frac{\partial \langle \tau_{ij} \rangle_\ell}{\partial x_i} - \frac{\partial T_{ij}}{\partial x_i} \quad (3)$$

$$\frac{\partial \langle \rho \rangle_\ell \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_i} = - \frac{\partial \langle J_i^\alpha \rangle_\ell}{\partial x_i} - \frac{\partial M_i^\alpha}{\partial x_i} + \langle \rho S_\alpha \rangle_\ell \quad (4)$$

where the scalar fields are denoted by $\phi_\alpha \equiv Y_\alpha$, $\alpha = 1, \dots, n_s$, and S_α is the production rate of species α . For $\alpha = n_s + 1$, $\phi_{n_s+1} \equiv h^s = \sum_{\alpha=1}^{n_s} h_\alpha^s Y_\alpha$, and $S_{n_s+1} = S^r + S^c$, where the superscripts r and c denote contributions from the heat release due to combustion, and compressibility effects and viscous dissipation, respectively. These source terms can be expanded as follows: $S^r = -\sum_\alpha \Delta h_\alpha^o S_\alpha$, where Δh_α^o is the enthalpy of formation of species α , and $S^c = \frac{1}{\rho} \left(\frac{\mathcal{D}p}{\mathcal{D}t} + \tau_{ik} \frac{\partial u_i}{\partial x_k} \right)$, where $\mathcal{D}/\mathcal{D}t$ denotes the material derivative, and τ_{ij} is the viscous stress tensor. Equations (2, 3, and 4) are closed by the constitutive relation,⁴⁰

$$\langle p \rangle_\ell \approx \langle \rho \rangle_\ell \mathcal{R} \langle T \rangle_L \sum_{\alpha=1}^{n_s} \frac{\langle Y_\alpha \rangle_L}{W_\alpha} \quad (5)$$

where $\mathcal{R}$ is the Universal Gas Constant, W_α is the molecular weight of species α and T is the temperature. τ_{ij} and J_i^α denote the viscous stress tensor and the scalar fluxes, respectively.

$$\langle \tau_{ij} \rangle_\ell \approx \langle \mu \rangle_\ell \left(\frac{\partial \langle u_i \rangle_L}{\partial x_j} + \frac{\partial \langle u_j \rangle_L}{\partial x_i} - \frac{2}{3} \frac{\partial \langle u_k \rangle_L}{\partial x_k} \delta_{ij} \right) \quad (6)$$

$$\langle J_i^\alpha \rangle_\ell \approx -\langle \rho \rangle_\ell \langle D \rangle_L \frac{\partial \langle \phi_\alpha \rangle_L}{\partial x_i} \quad (7)$$

where μ is the molecular coefficient of viscosity, and D is the molecular diffusion coefficient. The current formulation assumes equal diffusion among the species and heat, *i.e.* $Le_\alpha = Le = 1$. This is reasonable because errors associated with not modeling preferential diffusion effects in high Reynolds number turbulent reacting flows are expected to be small.⁴¹

The SGS closure problem is associated with $T_{ij} = \langle \rho \rangle_\ell (\langle u_i u_j \rangle_L - \langle u_i \rangle_L \langle u_j \rangle_L)$ and $M_i^\alpha = \langle \rho \rangle_\ell (\langle u_i \phi_\alpha \rangle_L - \langle u_i \rangle_L \langle \phi_\alpha \rangle_L)$, respectively denoting the SGS stresses and SGS fluxes. These closures are based on models well established in non-reacting flows.^{3,42–44} In this work, algebraic closures based on eddy viscosity and eddy diffusivity will be utilized. In compressible reacting flows, additional models are required for the filtered compressibility and viscous dissipation terms, *i.e.* $\langle \rho S^c \rangle_\ell$, and filtered reaction rates of the mass fractions, *i.e.* $\langle \rho S_\alpha \rangle_\ell$, $\alpha = 1, \dots, n_s$. The models for the former have presented a challenge and only few have been in use in RAS with mixed results.^{43,44} The models for the latter are provided by the FDF methods.

B. Scalar filtered mass density function

The SFMDF, denoted by F_ℓ , is formally defined as

$$F_\ell(\phi; \mathbf{x}, t) \equiv \int_{-\infty}^{+\infty} \rho(\mathbf{x}', t) \zeta(\psi, \phi(\mathbf{x}', t)) \mathcal{G}(\mathbf{x}' - \mathbf{x}) d\mathbf{x}' \quad (8)$$

$$\zeta(\psi, \phi(\mathbf{x}, t)) \equiv \delta(\psi - \phi(\mathbf{x}, t)) \equiv \prod_{\alpha=1}^{n_s} \delta(\psi_\alpha - \phi_\alpha(\mathbf{x}, t)) \quad (9)$$

where δ denotes the delta function and ψ denotes the sample space of the scalar array. The term ζ is the “fine-grained” density,^{22,45} hence Eq. (8) defines the SFMDF as the *mass weighted spatially filtered* value of the fine-grained density function. With the filter properties specified in the previous section, F_ℓ has all of the properties of a PDF.²² The SFMDF transport equation can be obtained by applying the above definitions to the unfiltered form of scalar transport

equation, Eq. (4). The result, after some algebraic manipulation, is

$$\begin{aligned}
\frac{\partial F_\ell(\boldsymbol{\psi}; \mathbf{x}, t)}{\partial t} + \underbrace{\frac{\partial \langle u_i(\mathbf{x}, t) | \boldsymbol{\psi} \rangle_\ell F_\ell(\boldsymbol{\psi}; \mathbf{x}, t)}{\partial x_i}}_{\text{Resolved and SGS transport}} &= \underbrace{\frac{\partial}{\partial x_i} \left(\langle \rho \rangle_\ell \langle D \rangle_L \frac{\partial}{\partial x_i} \left(\frac{F_\ell(\boldsymbol{\psi}; \mathbf{x}, t)}{\langle \rho \rangle_\ell} \right) \right)}_{\text{Molecular diffusion}} \\
- \underbrace{\sum_{\alpha}^{n_s+1} \sum_{\beta}^{n_s+1} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\left\langle \hat{\rho}(\phi) D \frac{\partial \phi_\alpha}{\partial x_i} \frac{\partial \phi_\beta}{\partial x_i} \middle| \boldsymbol{\psi} \right\rangle_\ell \frac{F_\ell(\boldsymbol{\psi}; \mathbf{x}, t)}{\hat{\rho}(\boldsymbol{\psi})} \right)}_{\text{Micromixing}} &- \underbrace{\sum_{\alpha}^{n_s} \frac{\partial}{\partial \psi_\alpha} \left(\left\langle \hat{\rho}(\phi) \hat{S}_\alpha(\phi) \middle| \boldsymbol{\psi} \right\rangle_\ell \frac{F_\ell(\boldsymbol{\psi}; \mathbf{x}, t)}{\hat{\rho}(\boldsymbol{\psi})} \right)}_{\text{Chemical reaction source term}} \\
+ \underbrace{\frac{\partial}{\partial \psi_{n_s+1}} \left(\left\langle \hat{\rho}(\phi) \sum_{\alpha}^{n_s} \Delta h_\alpha^o \hat{S}_\alpha(\phi) \middle| \boldsymbol{\psi} \right\rangle_\ell \frac{F_\ell(\boldsymbol{\psi}; \mathbf{x}, t)}{\hat{\rho}(\boldsymbol{\psi})} \right)}_{\text{Heat release source term}} &- \underbrace{\frac{\partial}{\partial \psi_{n_s+1}} \left(\left\langle \left(\frac{Dp}{Dt} + \tau_{ik} \frac{\partial u_i}{\partial x_k} \right) \middle| \boldsymbol{\psi} \right\rangle_\ell \frac{F_\ell(\boldsymbol{\psi}; \mathbf{x}, t)}{\hat{\rho}(\boldsymbol{\psi})} \right)}_{\text{Compressibility effects}}
\end{aligned} \tag{10}$$

The above transport equation for the SFMDF contains conditionally filtered terms that are unclosed. These terms are the resolved and SGS transport, micromixing, and the compressibility effects. The respective models for these terms utilize the conventional gradient diffusion, and the interaction by exchange with the mean (IEM) model.⁴⁶ In the first generation FDF models, the resolved pressure fluctuations are assumed dominant, and the compressibility effects are assumed negligible *within the subgrid*. This assumption allows us to remove the conditional filtering operations from both the chemical source terms and the compressible effects term. Recent FDF models of Nik et al.,³¹ based on previous work in RAS of Delarue and Pope,⁴⁷ consider a fully coupled velocity-scalar-pressure joint FDF for LES of compressible reacting flows thereby accounting for compressibility effects within the subgrid. With the above modeling assumptions the transport equation for the SFMDF becomes,

$$\begin{aligned}
\frac{\partial F_\ell(\boldsymbol{\psi}; \mathbf{x}, t)}{\partial t} + \underbrace{\frac{\partial \langle u_i(\mathbf{x}, t) | \boldsymbol{\psi} \rangle_\ell F_\ell(\boldsymbol{\psi}; \mathbf{x}, t)}{\partial x_i}}_{\text{Resolved transport}} &= \underbrace{\frac{\partial}{\partial x_i} \left(\langle \rho \rangle_\ell (\langle D \rangle_L + D_t) \frac{\partial}{\partial x_i} \left(\frac{F_\ell(\boldsymbol{\psi}; \mathbf{x}, t)}{\langle \rho \rangle_\ell} \right) \right)}_{\text{Molecular diffusion and SGS transport (modeled as SGS diffusion)}} \\
- \underbrace{\sum_{\alpha}^{n_s+1} \frac{\partial}{\partial \psi_\alpha} \left(\Omega_m (\psi_\alpha - \langle \phi_\alpha \rangle_L) F_\ell(\boldsymbol{\psi}; \mathbf{x}, t) \right)}_{\text{Micromixing}} &- \underbrace{\sum_{\alpha}^{n_s} \frac{\partial}{\partial \psi_\alpha} \left(\hat{S}_\alpha(\boldsymbol{\psi}) F_\ell(\boldsymbol{\psi}; \mathbf{x}, t) \right)}_{\text{Chemical reaction source term}} \\
+ \underbrace{\frac{\partial}{\partial \psi_{n_s+1}} \left(\sum_{\alpha}^{n_s} \Delta h_\alpha^o \hat{S}_\alpha(\boldsymbol{\psi}) F_\ell(\boldsymbol{\psi}; \mathbf{x}, t) \right)}_{\text{Heat release source term}} &- \underbrace{\frac{1}{\langle \rho \rangle_\ell} \left(\frac{\partial \langle p \rangle_\ell}{\partial t} + \langle u_k \rangle_L \frac{\partial \langle p \rangle_\ell}{\partial x_k} + \langle \tau_{ik} \rangle_\ell \frac{\partial \langle u_i \rangle_L}{\partial x_k} \right) \frac{\partial F_\ell(\boldsymbol{\psi}; \mathbf{x}, t)}{\partial \psi_{n_s+1}}}_{\text{Compressibility effects}}
\end{aligned} \tag{11}$$

where D_t is the subgrid diffusivity, Ω_m is the frequency of mixing within the subgrid, and the terms due to chemical reactions appear in a closed form. The above equation can be integrated to obtain transport equations for the scalar moments. The equations for the first Favré moment, $\langle \phi_\alpha \rangle_L$, and the generalized variance, $\sigma_\alpha^2 = \langle \phi_\alpha^2 \rangle_L - \langle \phi_\alpha \rangle_L^2$ are:

$$\frac{\partial \langle \rho \rangle_\ell \langle \phi_\alpha \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L \langle \phi_\alpha \rangle_L}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\langle \rho \rangle_\ell (\langle D \rangle_L + D_t) \frac{\partial \langle \phi_\alpha \rangle_L}{\partial x_i} \right) + \langle \rho \rangle_\ell \langle S_\alpha \rangle_L \tag{12}$$

$$\begin{aligned}
\frac{\partial \langle \rho \rangle_\ell \sigma_\alpha^2}{\partial t} + \frac{\partial \langle \rho \rangle_\ell \langle u_i \rangle_L \sigma_\alpha^2}{\partial x_i} &= \frac{\partial}{\partial x_i} \left(\langle \rho \rangle_\ell (\langle D \rangle_L + D_t) \frac{\partial \sigma_\alpha^2}{\partial x_i} \right) + 2 \langle \rho \rangle_\ell \langle D \rangle_L \frac{\partial \langle \phi_\alpha \rangle_L}{\partial x_i} \frac{\partial \langle \phi_\alpha \rangle_L}{\partial x_i} \\
&+ 2 \langle \rho \rangle_\ell D_t \frac{\partial \langle \phi_\alpha \rangle_L}{\partial x_i} \frac{\partial \langle \phi_\alpha \rangle_L}{\partial x_i} - 2 \Omega_m \langle \rho \rangle_\ell \sigma_\alpha^2 + 2 \langle \rho \rangle_\ell (\langle \phi_\alpha S_\alpha \rangle_L - \langle \phi_\alpha \rangle_L \langle S_\alpha \rangle_L)
\end{aligned} \tag{13}$$

C. Stochastic system

The most convenient means of modeling and solving the FDF transport equation is via the stochastic differential equations (SDEs)^{48,49} and the Lagrangian Monte Carlo (MC) procedure,⁵⁰ respectively.^{22,24} The basis of this procedure

is the same as in other recent RAS^{51–54} and LES.^{31,33,55–58} Therefore, only some of the fundamental properties of the methodology will be described below. With the Lagrangian procedure, the FDF is represented by an ensemble of computational stochastic elements (or particles) which are transported in the physical space by the combined actions of convection and diffusion (molecular and turbulent). In addition, transport in the scalar composition space occurs due to chemical reaction, micromixing, and compressibility effects. These physical processes are described by the set of SDEs. The stochastic diffusion process is considered for this purpose,

$$d\mathcal{X}_i(t) = m_i(\mathcal{X}(t), t)dt + \Sigma_{ij}(\mathcal{X}(t), t)dW_j \quad (14)$$

where $\mathcal{X}_i$ is a vector of $i = 1, \dots, n$ diffusion processes, m_i is the drift vector, Σ_{ij} is the diffusion tensor, and W_j ($j = 1, \dots, m$) denotes the Wiener-Lévy processes (random walk). The SDEs used here are

$$dx_i^+ = \left(\langle u_i \rangle_L + \frac{1}{\langle \rho \rangle_\ell} \frac{\partial \langle \rho \rangle_\ell (\langle D \rangle_L + D_t)}{\partial x_i} \right) dt + \sqrt{2(\langle D \rangle_L + D_t)} dW_i \quad (15)$$

$$d\phi_\alpha^+ = (-\Omega_m (\phi_\alpha^+ - \langle \phi_\alpha \rangle_L) + S_\alpha(\phi^+)) dt, \quad \alpha = 1, 2, \dots, n_s \quad (16)$$

$$\begin{aligned} d\phi_{n_s+1}^+ = & \left(-\Omega_m (\phi_{n_s+1}^+ - \langle \phi_{n_s+1} \rangle_L) - \sum_{\alpha}^{n_s} \Delta h_\alpha^o \hat{S}_\alpha(\phi^+) \right) dt \\ & + \frac{1}{\langle \rho \rangle_\ell} \left(\frac{\partial \langle p \rangle_\ell}{\partial t} + \langle u_k \rangle_L \frac{\partial \langle p \rangle_\ell}{\partial x_k} + \langle \tau_{ik} \rangle_\ell \frac{\partial \langle u_i \rangle_L}{\partial x_k} \right) dt \end{aligned} \quad (17)$$

where the x^+ and ϕ^+ denote Lagrangian position and scalar value, respectively. The Fokker-Planck equation corresponding to Eqs. (15-17) is equivalent to Eq. (11).²² Thus, the solution of these SDEs represents the single-point FDF in the probabilistic sense. The above formulation has two disadvantages: first, it is unable to model the effects of preferential species and heat diffusion, and second, it gives rise to a spurious production of scalar variance (*i.e.* second term on the right hand side of Eq. (13)). Both of these issues have been addressed by the work of McDermott and Pope.⁵⁹

D. Numerical Procedure

The FDF is solved via a hybrid Eulerian and Lagrangian MC procedure.^{51,53,60} For a numerical solution of the Eulerian field, structured or unstructured, finite-difference or finite-volume (or other) approaches can be utilized. The coupling between the Eulerian solver and the Monte Carlo procedure is enacted via the source terms in the sensible enthalpy transport equation which is redundantly solved by the hybrid solver.

The MC solver provides the Favré averaged scalar fields by considering a set of n_p particles that evolve according to the SDEs described by Eqs. (15-17). Each particle carries the information pertaining to its position $x_i^{(n)}$ and scalar value, $\phi_\alpha^{(n)}$ for $n = 1 \dots n_p$. The simplest way of performing the temporal integration of SDEs is via the Euler-Maruyama approximation^{49,50}

$$\mathcal{X}_i^{(n)}(t_{k+1}) = \mathcal{X}_i^{(n)}(t_k) + m_i^{(n)}(\mathcal{X}(\mathbf{t}_k), t_k) \Delta t + \Sigma_{ij}^{(n)}(\mathcal{X}(t_k), t_k) \Delta t^{\frac{1}{2}} \xi_j^{(n)}(t_k) \quad (18)$$

where $\xi^{(n)}(t_k)$ is an independent standardized Gaussian random variable. Additionally, the temporal integration is performed using a splitting technique which is necessary to facilitate integration of the stiff chemical source terms. That is, first, the scalar values of each particle are updated via a mixing model, and second, the chemical source terms are integrated using the updated scalar values as initial condition. This simple two-step process is shown to be first-order accurate, although higher order splitting approaches have also been recently developed.⁶¹ To understand the operational procedures of the hybrid configuration, the elements of the computation are shown in Fig. 1.

This figure shows the MC particles randomly distributed and freely moving within the computational domain. The particle transport is Lagrangian; thus the solution is free of constraints associated with typical convection on fixed grid points. Statistical information is obtained by considering an ensemble of n particles residing within each computational cell volume. The transfer of information from cells to the MC particles is accomplished via interpolations.

To reduce the computational cost and maintain statistical accuracy in variable density flows, the MC particles enter the computational domain uniformly but carry a weight (ω) that is proportional to the density at the inflow. The Favré

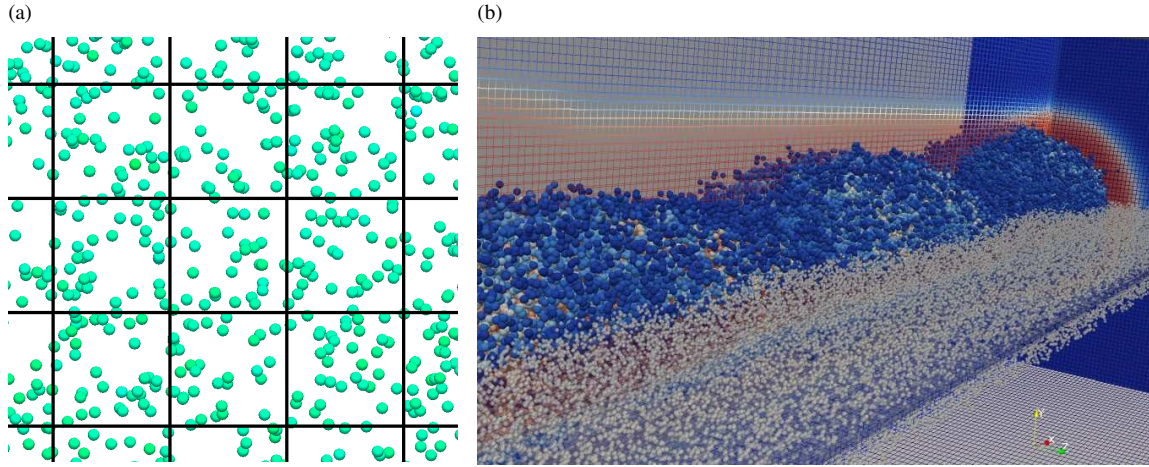


Figure 1. Hybrid numerical procedure. (a) Two dimensional schematic of the elements involved in computation using a typical hybrid Eulerian-Lagrangian solver. Black boxes denote the computational cells, and circles the Lagrangian particles, respectively. (b) Three dimensional hybrid simulation illustrating Lagrangian particles being convected over Cartesian grid. The colors of the particles denote their scalar values.

averaged value of a quantity $\hat{Q}(\phi(\mathbf{x}, t))$ is then obtained by a weighted average

$$\overline{\hat{Q}(\phi(\mathbf{x}, t))} \approx \frac{\sum_{n \in (\Delta)^3} \omega^{(n)} \hat{Q}(\phi^{(n)})}{\sum_{n \in (\Delta)^3} \omega^{(n)}} \quad (19)$$

Particle cloning and clustering strategies are also employed.⁵³ These strategies add and remove stochastic particles, respectively, in areas of the flow where the particle number density exceeds predefined lower and upper limits. In steady-state RAS/PDF methods, a variable time-stepping algorithm can also be utilized to accelerate the convergence of the MC simulation.⁶² The consistency of the hybrid numerical approach is evaluated by comparing the ensemble averaged means (or variances) of the scalar variables, since these quantities can be solved independently by the Eulerian and Lagrangian solvers.

III. Particle tracking

One of the key numerical elements of the hybrid FDF solver is an efficient particle tracking algorithm. This is because a typical hybrid FDF simulation will require a minimum of about 20 MC particles per computational cell for accuracy.⁶⁰ Given that a high fidelity LES of a practical high-speed combustor device will currently utilize about 10-100 million computational cells, the number of MC particles can reach 0.2-2 billion. There are two aspects related to efficiency: first, the mathematical formulation of the tracking algorithm itself; second, the efficient, parallelizable, and scalable numerical implementation. The tracking algorithms can range from readily parallelizable cell-index identification methods applicable only on uniform Cartesian meshes^{63,64} to methods utilizing near-neighbor search applicable on unstructured meshes.⁶⁵ An efficient and robust compromise between these two, that is also applicable to complex geometries and both structured and unstructured grids, is a convex polyhedron method developed by Pope and described in detail by Subramaniam and Haworth.⁶⁶ This method is similar to one used by Ansari et al.,⁶⁵ however it does not require the near-neighbor search because the particles are always partially advected to the cell faces first. Since the cell faces contain information about their neighbors the advection can continue for the remainder of the particle time step inside the correctly identified cell without the need for a search. Because near neighbor searches are computationally expensive, this search-less algorithm can potentially lower the computational costs associated with particle tracking. The approach of Subramaniam and Haworth⁶⁶ is also robust because it does not require that the particle convective Courant-Friedrichs-Lewy (CFL) number be less than one. Such a requirement is often enforced when near-neighbor search algorithms are employed to limit the extent of the search domain. Furthermore, particle CFL requirements may be misleading. This is because the particle CFL number is typically defined based on some characteristic length, *e.g.* minimum cell edge length. Independently of such definition, particles can still traverse

multiple cells along the cell corners even in the limit of the particle CFL number approaching zero. This could result in a numerical “loss-of-tracking” of particles, and more importantly, loss of mass conservation in the Lagrangian simulation causing errors that are much larger than those associated with truncation errors of the Lagrangian solver. Stopping particles at the cell faces as proposed by Subramaniam and Haworth⁶⁶ introduces additional modeling benefits in flows with flow discontinuities and in multiphase flows. In the former, since the particles’ advection properties (e.g. velocities) are updated at the cell faces, the particle can respond to compressible flow features (such as shocks) as soon as they are encountered. In the latter, the mass associated with evaporating fuel from the Lagrangian droplet can be accurately assigned to the corresponding Eulerian cells in which evaporation occurred.

IV. Coupling LES/FDF with RAS/PDF

Predictions of high Reynolds number, wall-bounded flows remain a challenge for LES because the grid size requirements necessary to resolve the turbulent boundary layer are on the order of those required for the corresponding DNS.⁶ This requirement is less severe in RAS because only the wall-normal direction must be “resolved” for accurate near-wall solutions. Furthermore, RAS has benefited from several decades of near-wall modeling efforts which resulted in the development of models that allow for the reduction of wall-normal grid spacing without significant loss in predictive accuracy.⁴³ Given the benefits of RAS it seemed natural to develop hybrid LES/RAS methods for LES of wall-bounded flows.⁶⁷ While there is no reason to expect that the wall-models developed for non-reacting RAS will perform well in near-wall turbulent, reacting flows, the hybrid LES/FDF-RAS/PDF method with the wall-normal directions resolved should be a good candidate for such simulations. This is because such a hybrid model would allow for high fidelity modeling of a flame near and through the turbulent boundary layer.

The turbulent flame-wall interactions (FWI) are of considerable importance when designing practical combustor devices. This is because these interactions have a major impact on both the mean and maximum heat fluxes to the wall. The former guides the cooling requirements, and the latter impacts the lifetime of a combustor. The mechanisms of FWI are somewhat understood and recent DNS data are available.⁶⁸ Two canonical configurations are typically considered: First is the head-on-quenching (HOQ), where the flame front travels perpendicularly to the wall and impinges on it causing flame quenching leading to maximum heat flux. Second is the side-wall quenching (SWQ), where the flame front travels parallel to the wall with the quenching of the flame front edge nearest to the wall. Also, in both low and high speed boundary layer flows, the flame propagation inside the boundary layer may cause flashback, i.e. upstream propagation of the flame-front through the low velocity boundary layer regions. While, flashback is unlikely in high-speed boundary layers with favorable pressure gradients, when the boundary layer is weakened by adverse pressure gradient and/or impinging shock, flashback may become possible. Furthermore, if during such shock-boundary-layer interactions (SBLI) the shock impinges on a boundary layer containing a premixed fuel-air mixture then ignition may occur causing localized peak heat fluxes that are much larger than those due to SBLI alone.

The ability to model turbulent FWI has the potential to improve predictions of not only internal reacting flows but also external hypersonic flows such as flows over hypersonic vehicle bodies and reentry vehicles. Duan and Martín⁶⁹ have shown that modeling turbulence-chemistry interactions inside the boundary layers of dissociating air may be important to improve predictions of high enthalpy external flows. The coupling of the hybrid LES/FDF-RAS/PDF method could be achieved by utilizing a blending function of the transport parameters. However, further research is required to determine the form of such a blending function as the reacting boundary layer is likely to exhibit non-universal behavior.

V. Accelerating chemistry

A. Flamelet Generated Manifolds for compressible flows

Simulating detailed chemistry in reacting flows requires significant computational resources because chemical source terms are highly non-linear and numerically stiff. Direct integration using a detailed reaction mechanism in LES or hybrid LES/RAS is currently computationally intractable for flows typically found within a scramjet combustor because the necessary additional computational resources render such simulations too expensive for geometries of practical interest. That being said, recent advances by the authors toward massively scalable implementations of LES/FDF using detailed chemistry and utilizing petascale platforms show great potential and will be discussed in the following section. Nevertheless, in order to make substantial progress toward the simulation of high-speed combusting flows, simulations must be performed using less-expensive, but similarly accurate, treatments of the finite-rate

chemistry. Several methods have been proposed for reducing the complexity of finite-rate kinetics, including: reducing reaction mechanisms using sensitivity analyses,^{70,71} dynamic tabulation and look-up of relevant chemical quantities using the in-situ adaptive tabulation (ISAT) approach,⁷² and pre-tabulation of relevant chemical quantities using a flamelet-derived method³⁶ that combines the advantages of laminar flamelets⁷³ and the Intrinsic Low Dimensional Manifold (ILDM) method.⁷⁴ However, these current methods are inadequate for supersonic combustion, in which compressibility, pressure, and turbulence effects play a significant role in the combustion physics.

Flamelet-generated manifolds (FGM) have been used extensively as a means of simulating low-Mach number combustion due to their inherent compatibility with varying-complexity reaction mechanisms and drastic reduction in simulation runtime.^{36,75} In its most-general form, FGM reduces detailed chemistry to a low-dimensional manifold in composition space parameterized by a reduced set of controlling variables. Prior to simulation, a set of one-dimensional laminar counter-flow flames are solved with varying initial conditions, and a table is constructed by parameterizing the flamelet solutions by mixture fraction and a reaction progress variable. During simulation, transport equations for the mixture fraction and progress variable are solved, in addition to those for the mass, momentum, and energy. At each integration step, the transported mixture fraction and progress variable are used to lookup chemical quantities from the table, such as chemical composition data, required to integrate the energy equation forward in time.

The development of the flamelet equations requires several limiting assumptions, including: incompressibility (low Mach number), constant pressure, and steady-state.³⁶ Thus, the validity of these equations diminishes for highly-compressible supersonic combustor flows. Recently, various methods for modifying the FGM approach to include pressure, compressibility, and unsteady effects have been proposed in the literature, and several approaches are described briefly here. Bekdemir et al.⁷⁶ simulated diesel engine combustion using the FGM approach in which flamelet solutions were parameterized by mixture fraction, a progress variable, and pressure. Flamelets were computed and tabulated for seven pressure levels ranging from the pressure at fuel injection to the point of maximum pressure. A pressure-dependency study indicated that a minimum of five logarithmically-distributed pressure levels were necessary to adequately represent pressure variation through compression and combustion. However, averaged results from the FGM simulations indicated artificially-high pressure rises as a consequence of unrealistic short burn durations. Based on these findings, the researchers suggested future work include: better capture of the strain rate dependency of ignition and investigation into using both premixed and non-premixed flamelet solutions. Although this work focused on subsonic combustion, the notion of adding pressure as an additional dimension to an FGM may prove useful for the case of supersonic combustion.

Rather than parameterize the FGM table by pressure, Emory et al.⁷⁷ attempted to include the effects of compressibility and pressure on the simulation for the HyShot II hydrogen-fueled scramjet experiment by imposing a pressure-dependent scaling on the progress variable source term. Rather than use the temperature corresponding to the flamelet solutions, the transported total energy was used to derive an analytical formulation for temperature by first approximating the total energy according to Eq. 20 and then linearly expanding in temperature the ratio of specific heats around the tabular value in Eq. 21. Performing the integration analytically in Eq. 20 and rearranging yielded the closed-form approximation for temperature included in Eq. 22. Without this linearization, a Newton-Raphson method would be required to solve for the temperature. The effect of pressure on the combustion is approximated using a scaling on the progress variable source term. Since the combustion of hydrogen is governed primarily by bimolecular reactions, the researchers approximated the progress variable source term according to Eq. 23, in which the source term computed at a reference pressure is scaled by the square of the normalized pressure to yield a pressure-dependency. Simulations at various equivalence ratios for the HyShot II experiment indicated qualitative agreement with experimental data.

$$E = E_0 + \int c_v dT = E_0 + \int \frac{R_0}{\gamma - 1} dT \quad (20)$$

$$\gamma = \gamma_0 + a_\gamma(T - T_0) \quad (21)$$

$$T = T_0 + \frac{\gamma_0 - 1}{a_\gamma} [e^{\frac{a_\gamma(E - E_0)}{R}} - 1] \quad (22)$$

$$\dot{\omega}_C = \left(\frac{p}{p_{ref}} \right)^2 \dot{\omega}_{C,ref} \quad (23)$$

Lacaze and Oefelein⁷⁸ performed a detailed study on the use of flamelets for modeling non-premixed combustion at supercritical pressures for simulations of rocket engines, where pressures exceed 50 atm. Detailed opposed-jet hydrogen-air flame calculations found that: 1) the flame was thin and robust over a wide range of strain rates, 2) the flame structure in mixture fraction space was approximately independent of pressure, 3) within the reaction zone, temperature had little effect on flame structure, and 4) the heat release was sensitive to pressure and strain fluctuations. Based on these findings, the researchers devised an FGM approach for compressible reacting flow simulations within the supercritical pressure regime based on coupling the total non-chemical energy transport equation and table through a modified chemical source term. Pressures experienced during supersonic combustion within a scramjet are not supercritical and typically range from 0.5-5.0 atm with significant flame strain effects. Thus, the results of Lacaze and Oefelein⁷⁸ maybe of limited use for such flows.

Though attempts have been made at including compressible and pressure effects in the FGM framework, current methods are still ill-equipped to simulate the strongly unsteady, compressible phenomena comprising dual-mode scramjet combustion. Within this flow regime, higher-fidelity implementations of FGM that include more robust transport equation-table couplings and detailed pressure and compressibility effects will be necessary. To further ascertain unsteady, turbulence-driven flow properties, such a high-fidelity FGM approach will likely necessitate an LES or hybrid LES/RAS solution framework.

B. Irregularly Portioned Lagrangian Monte Carlo Finite Difference for scalable reacting simulations with finite-rate chemistry

Petascale computing has been a reality for open research for the past couple of years, and the exascale platforms are the current technological trend which are expected to be available by the end of this decade.⁷⁹ Being able to take advantage of the enormous opportunity of such extreme scale computing platforms is vital to the success of LES and its application in industrial practice.

Design and implementation of scalable parallel algorithms is the key enabler in the petascale arena. However, this is not a trivial task, especially in LES of reacting flows where complex chemistry calculations typically dominate the computation. The issue is further exacerbated by the dynamic and inhomogeneous nature of the flow. The variation in composition affects the level of stiffness of the chemistry equations. These variations cause the computational load to vary significantly throughout the solution domain, which negatively impacts the duration of a simulation. This phenomena has been observed in reacting computations with detailed or reduced chemistry via direct integration and may also be relevant to acceleration techniques discussed in the previous section. The impact of it is made evident in Fig. 2 which shows the variation in the computational load at some instant during the simulation of Sandia flame D,⁸⁰ using direct integration. It is observed that the computational requirement is highly non-uniform throughout; virtually no time is spent for calculations near the cold jet or the cold surrounding air, and most of the computational load is concentrated around the hot pilot.

This nature of reacting flow renders straightforward parallelization techniques ineffective, limiting scalability at only 100s of computing units as will be shown. An effective parallelization must be adaptive and be driven by the dynamics of the flow. We have developed and implemented such a methodology for LES/FDF, termed “Irregularly Portioned Lagrangian Monte Carlo Finite Difference” (IPLMCFD). This is a dynamic load balancing technique that is especially effective for structured mesh configurations, but is also applicable in a straightforward manner for unstructured meshes. It allows for efficient LES of reacting flow on thousands of computing units, and in the context of FDF, has a potential to scale to hundreds of thousands of computing units by readily being able to take advantage of the heterogeneous multicore nature of today’s petascale systems.

A popular parallelization strategy in modern CFD is via temporally invariant block decomposition where the mesh is partitioned into equally sized boxes, and each box is assigned to a processor (Fig. 3(a)). This uniformity is relatively easy to implement and yields a minimal communication overhead. But for unsteady and inhomogeneous flows, it usually leads to a poor load distribution. Processors with lighter loads must wait (and remain idle) until the synchronization at the end of each time step. The local computation time of each processor for this is shown in Fig. 3(c). In this example, the idle time is about half of the total time. We show that the load imbalance problem can be fully resolved by portioning the domain *irregularly and adaptively*. In doing so, the Eulerian mesh is represented as an undirected graph where particle cells are the vertices of the graph and are weighted by the computational load. Each vertex is assigned a computational weight, *i.e.* a computation-load metric, which is a function of heterogeneous and homogeneous computational loads. This weighted graph is then fed into a graph partitioning algorithm⁸¹ which subdivides the domain into clusters of particle cells on which the computational load is evenly distributed. Figure 3(d)

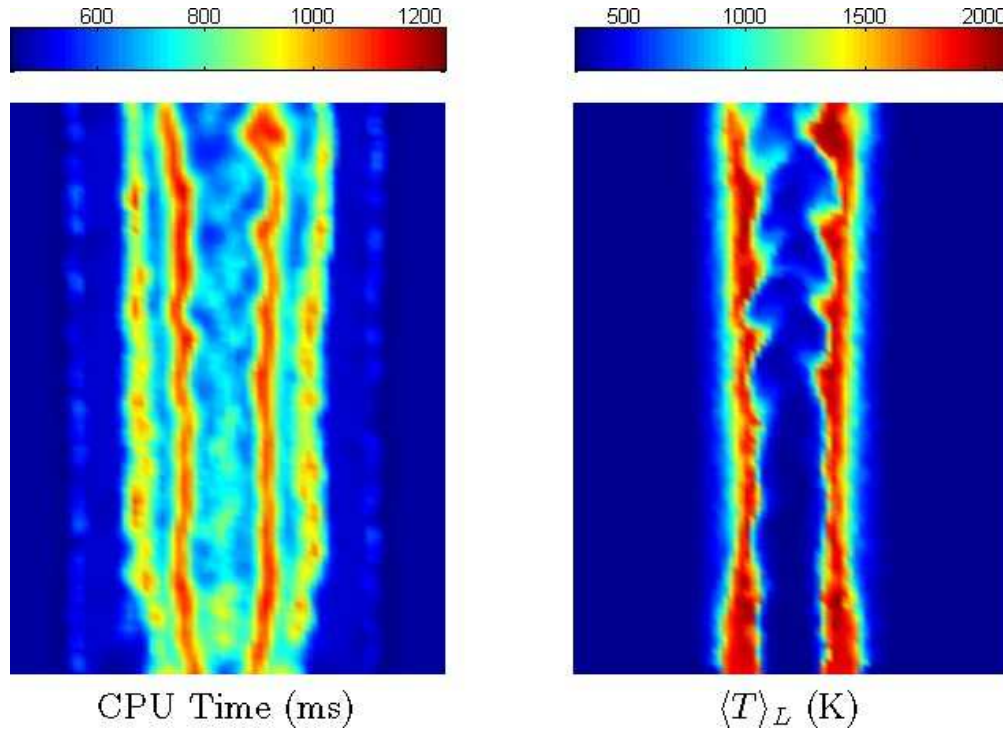


Figure 2. Instantaneous CPU time in milliseconds spent performing particle integrations (left). Instantaneous filtered temperature (right).

shows the load distribution corresponding to the balanced irregular decomposition. Here, the idle time is insignificant. The transient load re-distribution problem is envisioned to be resolved by recomputing the load metric, repartitioning the domain, and intercommunicating the local data of the partitions as the simulation proceeds. The frequency of re-distribution is adjusted based on the communication cost and the extent of load imbalance. The issue of local data migration required for such a dynamic load balancing without sacrificing scalability has been investigated by many, *e.g.* see Devine et al.⁸². Furthermore, software such as Zoltan⁸³ can readily deal with this issue.

Our current implementation of IPLMCFD for LES/FDF employs the message passing interface (MPI) for distributed parallelism via inter-partition communication, and can scale up to 1000s of partitions via the adaptive partitioning as described. From Fig. 4, it is evident that the IPLMCFD methodology outperforms uniform decomposition. Not shown on the plot are the actual walltimes. In particular, the sequential run for this configuration takes about 3,000 seconds *per iteration*[¶]; with 256 processors, uniform partitioning has $45/250 = 18\%$ scalability with 66.7 seconds per time step, whereas IPLMCFD soars at 97% scalability bringing down the walltime to 11.4 seconds. In other words, a mere load balancing with the same amount of resources provides almost a 6 fold increase in computational throughput! By moving into the thousands of processors range an unbalanced decomposition is simply not feasible. IPLMCFD scales almost ideally up to 4000 processors, and starts to tail off slightly beyond this limit as the effects of communication become more and more pronounced. Nevertheless, for such a moderately sized simulation, it performs favorably. It is important to emphasize that in strong scalability analyses, the size of the simulation is kept fixed for all processors. We project this tailing-off to surpass 10,000 processors for larger simulations with which the data-to-communication ratio is much higher. This and, other weak scaling properties will be discussed in a future publication.⁸⁴

Ability to utilize $\mathcal{O}(10^4)$ processors effectively in order to conduct LES of laboratory scale flames within hours, instead of months, has been a major step forward. However, ten thousand processors do not qualify as “petascale,” and will be rather insufficient given that our objective is to be able to conduct much larger, realistic, and industry scale simulations quickly. It is important to emphasize once again that the analysis shown thus far has been for purely message passing, single processor-core per partition runs. The next phase of improvements will substantiate from recognizing

[¶]The mesh size for this analysis is moderate enough to allow for sequential runs; otherwise, in a more realistic geometry and mesh size, memory and time constraints would be prohibit a sequential run.

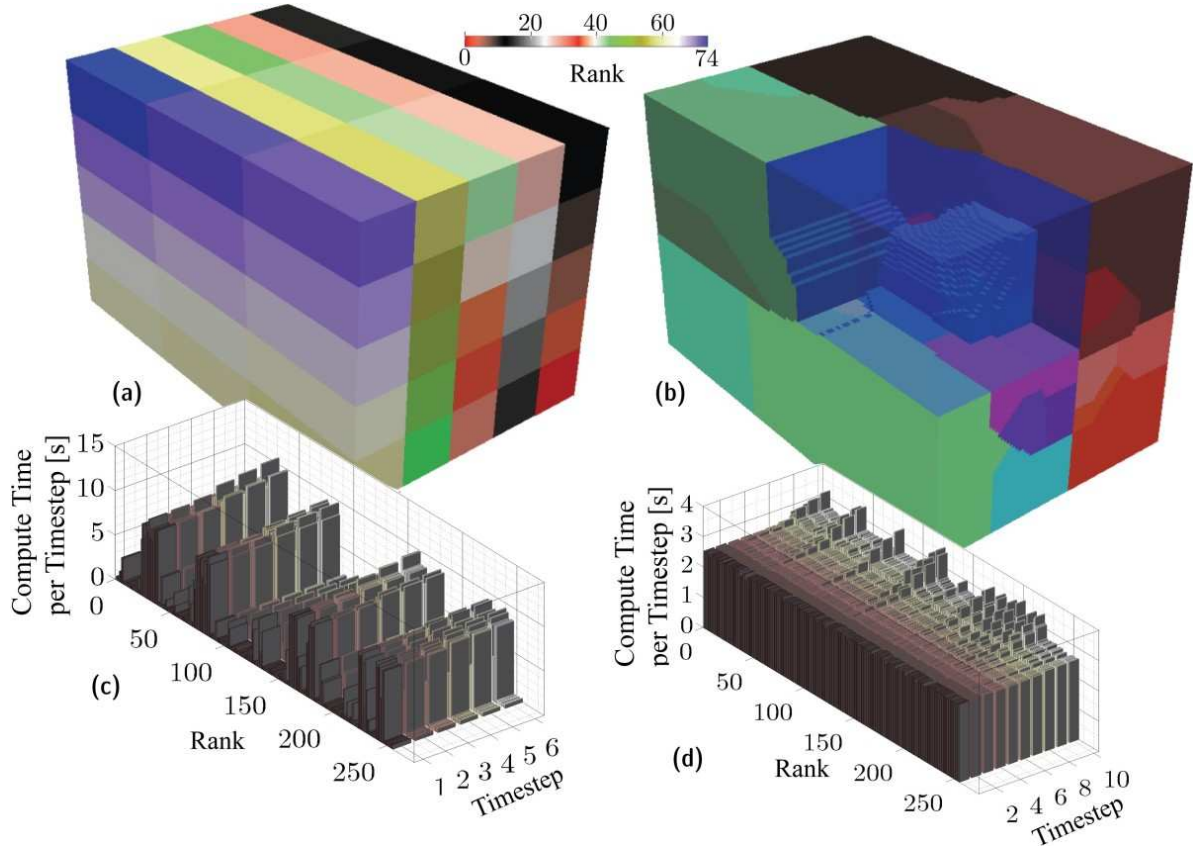


Figure 3. Domain topology with (a) the uniform decomposition, and (b) adaptive irregular decomposition. Non-idle CPU times per time-step for each rank for subsequent time-steps with (c) uniform decomposition, and (d) adaptive irregular decomposition.

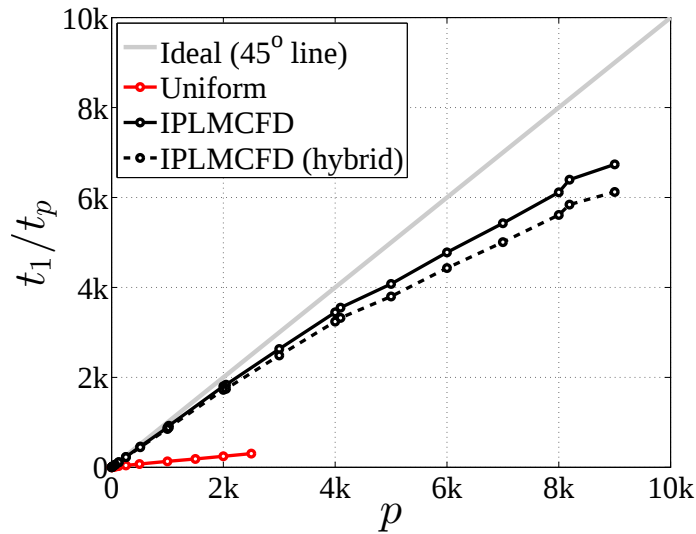


Figure 4. Ratio of serial-to-parallel simulation time versus the number of processors demonstrates the strong scaling results for IPLMCFD in comparison with those obtained with uniform decomposition. Also shown is the scaling result for single partition per compute node (hybrid). These analyses are conducted on Kraken, the supercomputer at the National Institute for Computational Sciences (NICS), Knoxville, TN.

the trend in today's supercomputing: *petascale computers are becoming predominantly heterogeneous in nature*⁸⁵ ||.

As discussed in Section II.D., MC simulations typically require order of millions to billions of particles; moreover, as indicated in Section V.A., the evaluation of chemistry equations, Eqs. (16), and (17) is computationally the most significant portion of per partition workload. With a balanced distribution of particle workload to separate and independent partitions, a further local refinement can be made whereby the work for local ensembles of MC particles can be split out to individual CPU cores and/or graphical processing units (GPUs), using shared memory parallelism (for example, via OpenMP⁸⁶), and general purpose GPU programming (for example, via NVIDIA/CUDA⁸⁷ or OpenCL⁸⁸), respectively. Given thread-safe and GPU based implementations of chemistry and stiff-solver routines, such fine grained parallelism can be implemented scalably in a straightforward fashion. This is an active area of research, and some example implementations are available in the literature.^{89,90} These efforts, in combination with the virtually unbounded, distributed, parallel scalability enabled by IPLMCFD, will provide numerical frameworks which are able to leverage petascale platforms effectively for high-fidelity and highly reliable LES of industry scale applications.

VI. Conclusions

The scalar filtered mass density function (SF MDF) model for large eddy simulations (LES) of high speed reacting flows has been presented. The key benefit of this model is that the most challenging aspect of modeling the reacting flows (both low and high speed) namely the filtered reaction source terms appears in closed form. The current version of the model requires a unity Lewis number and introduces spurious production of scalar variance. Both issues have been resolved by modifications to this model. A less defensible assumption embedded in the current SF MDF is that of constant pressure within the subgrid. This, however, is addressed by the next generation model, the joint velocity-scalar-pressure filtered density function (FDF), although an intermediate joint scalar-pressure formulation may also be possible. To solve the FDF transport equation, a hybrid Eulerian-Lagrangian solver is utilized. The Eulerian solver integrates the continuity, momentum, and energy equations via a finite-difference or finite-volume (or other) method on either structured or unstructured grids. The Lagrangian solver integrates a set of stochastic differential equations using a Monte Carlo particle method. The key element of the latter is a robust, efficient, and parallelizable particle tracking algorithm based on the convex polyhedron method. To model turbulent flame wall interactions important to predicting mean and peak values of the wall heat flux, a coupling of LES/FDF with Reynolds averaged simulations (RAS) utilizing probability density function (PDF) method was also discussed. This approach is based on the hybrid LES/RAS model developed by Baurle et al.⁶⁷ The most computationally intensive component of any reacting simulation is the integration of finite-rate kinetics. To reduce the numerical costs associated with such integrations the flamelet generated manifold (FGM) model was proposed and discussed. Several challenges to applying FGM in high speed compressible flows have been identified. The main ones included the variable pressure effects, and unique parametrization of pure mixing states in compressible flows. For cases where finite-rate kinetics are desired, the computational costs of numerical integration can be significantly reduced by deploying the Irregularly Portioned Lagrangian Monte Carlo Finite Difference (IPLMCFD) method. The combination of modeling and numerical capabilities discussed in this paper have the potential to overcome the significant computational cost of utilizing FDF methods in practical applications.

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|| See <http://top500.org/list/2012/06/100> for June 2012 listing

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